N,N'-Diphenylformamidine

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 7.11e-03 mol/L

Global applicability domain: Inside

Local applicability domain index: 5.00e-01

Confidence level: 4.47e-01

Nearest Neighbors from the Training Set

Image not found
1,10-Phenanthroline
Measured: 1.49e-02
Predicted: 5.60e-03

Image not found
N-(1-Naphthyl)ethylenediamine
Measured: 1.07e-02
Predicted: 9.11e-02

Image not found
Quinoxaline
Measured: 5.07
Predicted: 1.30e-01

Image not found
1-Phenyl-2-thiourea
Measured: 1.62e-02
Predicted: 7.48e-02

Image not found
Heptachlor epoxide
Measured: 5.14e-07
Predicted: 3.52e-07